Advanced Crash Course in Supercomputing: Parallelism

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Outline

I. Parallelism
II. Supercomputer Architecture
III. Basic MPI
IV. MPI Collectives
V. Debugging and Performance Evaluation

I. PARALLELISM

Parallel Lines **by Blondie. Source:**
http://xponentialmusic.org/blogs/885mmmm/2007/10/09/403-blondie-hits-1-with-heart-of-glass/

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I. Parallelism

- Concepts of parallelization
- Serial vs. parallel
- Parallelization strategies

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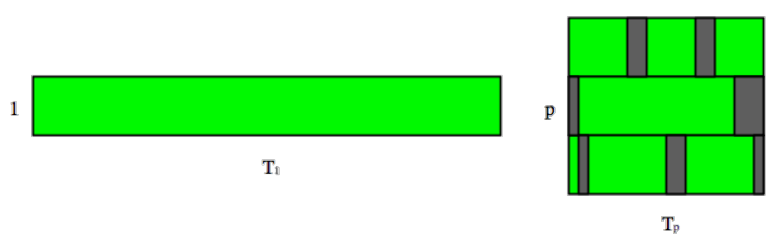
Parallelization Concepts

- When performing task, some subtasks depend on one another, while others do not
- Example: Preparing dinner
  - Salad prep independent of lasagna baking
  - Lasagna must be assembled before baking
- Likewise, in solving scientific problems, some tasks independent of one another

Serial vs. Parallel

- Serial: tasks must be performed in sequence
- Parallel: tasks can be performed independently in any order



Serial vs. Parallel: Example

- Example: Preparing dinner
  - Serial tasks: making sauce, assembling lasagna, baking lasagna; washing lettuce, cutting vegetables, assembling salad
  - Parallel tasks: making lasagna, making salad, setting table

Serial vs. Parallel: Example

- Could have several chefs, each performing one parallel task
- This is concept behind parallel computing

Parallel Algorithm Design: PCAM

- *Partition:* Decompose problem into fine-grained tasks to maximize potential parallelism
- *Communication:* Determine communication pattern among tasks
- *Agglomeration:* Combine into coarser-grained tasks, if necessary, to reduce communication requirements or other costs
- *Mapping:* Assign tasks to processors, subject to tradeoff between communication cost and concurrency

(taken from *Heath: Parallel Numerical Algorithms*)

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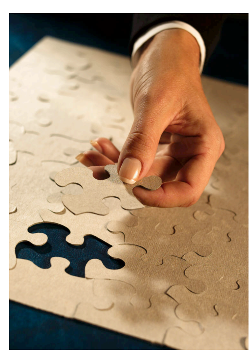
Discussion: Jigsaw Puzzle*

- Suppose we want to do 5000 piece jigsaw puzzle
- Time for one person to complete puzzle: n hours
- How can we decrease walltime to completion?



* Thanks to Henry Neeman

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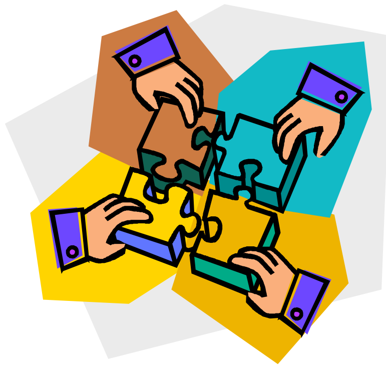
Discussion: Jigsaw Puzzle



- Add another person at the table
  - Effect on wall time
  - Communication
  - Resource contention
- Add p people at the table
  - Effect on wall time
  - Communication
  - Resource contention

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Discussion: Jigsaw Puzzle

- What about: p people, p tables, $5000/p$ pieces each?
- What about: one person works on river, one works on sky, one works on mountain, etc.?

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II. ARCHITECTURE

Image: Louvre Abu Dhabi – Abu Dhabi, UAE, designed by Jean Nouvel, from
http://www.inhabitat.com/2008/03/31/jean-nouvel-named-2008-pritzker-architecture-laureate/

II. Supercomputer Architecture

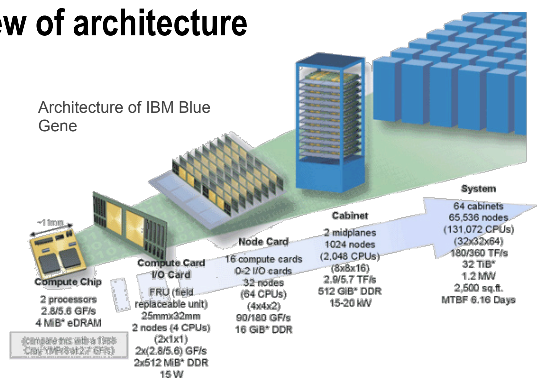
- What is a supercomputer?
- Conceptual overview of architecture

Cray 1
(1976)

IBM Blue
Gene
(2005)

Cray XT5
(2009)

Architecture of IBM Blue
Gene



What Is a Supercomputer?

- "The biggest, fastest computer right this minute." -- Henry Neeman
- Generally 100-10,000 times more powerful than PC
- This field of study known as *supercomputing, high-performance computing (HPC),* or *scientific computing*
- Scientists use really big computers to solve really hard problems

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SMP Architecture

- Massive memory, shared by multiple processors
- Any processor can work on any task, no matter its location in memory
- Ideal for parallelization of sums, loops, etc.

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Cluster Architecture

- CPUs on racks, do computations (fast)
- Communicate through myrinet connections (slow)
- Want to write programs that divide computations evenly but minimize communication

State-of-the-Art Architectures

- Today, hybrid architectures gaining acceptance
- Multiple {quad, 8, 12}-core nodes, connected to other nodes by (slow) interconnect
- Cores in node share memory (like small SMP machines)
- Machine appears to follow cluster architecture (with multi-core nodes rather than single processors)
- To take advantage of all parallelism, use MPI (cluster) and OpenMP (SMP) hybrid programming

III. MPI

MPI also stands for Max Planck Institute for Psycholinguistics. Source: http://www.mpi.nl/WhatWeDo/istitute-pictures/building

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III. Basic MPI

- Introduction to MPI
- Parallel programming concepts
- The Six Necessary MPI Commands
- Example program

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Introduction to MPI

- Stands for *M*essage *P*assing *I*nterface
- Industry standard for parallel programming (200+ page document)
- MPI implemented by many vendors; open source implementations available too
  - ChaMPIon-PRO, IBM, HP, Cray vendor implementations
  - MPICH, LAM-MPI, OpenMPI (open source)
- MPI function library is used in writing C, C++, or Fortran programs in HPC
- MPI-1 vs. MPI-2: MPI-2 has additional advanced functionality and C++ bindings, but everything learned today applies to both standards

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Parallelization Concepts

- Two primary programming paradigms:
  - SPMD (single program, multiple data)
  - MPMD (multiple programs, multiple data)
- MPI can be used for either paradigm

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SPMD vs. MPMD

- SPMD: Write single program that will perform same operation on multiple sets of data
  - Multiple chefs baking many lasagnas
  - Rendering different frames of movie
- MPMD: Write different programs to perform different operations on multiple sets of data
  - Multiple chefs preparing four-course dinner
  - Rendering different parts of movie frame
- Can also write hybrid program in which some processes perform same task

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The Six Necessary MPI Commands

- `int MPI_Init(int *argc, char **argv)`
- `int MPI_Finalize(void)`
- `int MPI_Comm_size(MPI_Comm comm, int *size)`
- `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
- `int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`
- `int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`

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Initiation and Termination

- `MPI_Init(int *argc, char **argv)` initiates MPI
  - Place in body of code after variable declarations and before any MPI commands
- `MPI_Finalize(void)` shuts down MPI
  - Place near end of code, after last MPI command

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Environmental Inquiry

- `MPI_Comm_size(MPI_Comm comm, int *size)`
  - Find out number of processes
  - Allows flexibility in number of processes used in program
- `MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - Find out identifier of current process
  - 0 ≤ `rank` ≤ `size`-1

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Message Passing: Send

- **`MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)`**
  - Send message of length `count` bytes and datatype `datatype` contained in `buf` with tag `tag` to process number `dest` in communicator `comm`
  - E.g. `MPI_Send(&x, 1, MPI_DOUBLE, manager, me, MPI_COMM_WORLD)`

Message Passing: Receive

- **`MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag, MPI_Comm comm, MPI_Status *status)`**
  - Receive message of length `count` bytes and datatype `datatype` with tag `tag` in buffer `buf` from process number `source` in communicator `comm` and record status `status`
  - E.g. `MPI_Recv(&x, 1, MPI_DOUBLE, source, source, MPI_COMM_WORLD, &status)`

Message Passing

- WARNING! Both standard send and receive functions are *blocking*
- `MPI_Recv` returns only after receive buffer contains requested message
- `MPI_Send` may or may not block until message received (usually blocks)
- Must watch out for deadlock

Deadlocking Example (Always)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
    int me, np, q, sendto;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);
    if (np%2==1) return 0;
    if (me%2==1) {sendto = me-1;}
    else {sendto = me+1;}
    MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
    MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
    printf("Sent %d to proc %d, received %d from proc %d\n", me,
      sendto, q, sendto);
    MPI_Finalize();
    return 0;
}
```

Deadlocking Example (Sometimes)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
    int me, np, q, sendto;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);
    if (np%2==1) return 0;
    if (me%2==1) {sendto = me-1;}
    else {sendto = me+1;}
    MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
    MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
    printf("Sent %d to proc %d, received %d from proc %d\n", me,
      sendto, q, sendto);
    MPI_Finalize();
    return 0;
}
```

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Deadlocking Example (Safe)

```
#include <mpi.h>
#include <stdio.h>
int main(int argc, char **argv) {
    int me, np, q, sendto;
    MPI_Status status;
    MPI_Init(&argc, &argv);
    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &me);
    if (np%2==1) return 0;
    if (me%2==1) {sendto = me-1;}
    else {sendto = me+1;}
    if (me%2 == 0) {
        MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
        MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
    } else {
        MPI_Recv(&q, 1, MPI_INT, sendto, sendto, MPI_COMM_WORLD, &status);
        MPI_Send(&me, 1, MPI_INT, sendto, me, MPI_COMM_WORLD);
    }
    printf("Sent %d to proc %d, received %d from proc %d\n", me, sendto, q,
    sendto);
    MPI_Finalize();
    return 0;
}
```

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Explanation: Always Deadlock Example

- Logically incorrect
- Deadlock caused by blocking `MPI_Recvs`
- All processes wait for corresponding `MPI_Sends` to begin, which never happens

Explanation: Sometimes Deadlock Example

- Logically correct
- Deadlock could be caused by `MPI_Sends` competing for buffer space
- Unsafe because depends on system resources
- Solutions:
  - Reorder sends and receives, like safe example, having evens send first and odds send second
  - Use non-blocking sends and receives or other advanced functions from MPI library (see MPI standard for details)

IV. MPI COLLECTIVES

"Collective Farm Harvest Festival" (1937) by Sergei Gerasimov. Source: http://max.mmlc.northwestern.edu/~mdenner/Drama/visualarts/neorealism/34harvest.html

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MPI Collectives

- Communication involving group of processes
- Collective operations
  - Broadcast
  - Gather
  - Scatter
  - Reduce
  - All-
  - Barrier

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Broadcast

- Perhaps one message needs to be sent from manager to all worker processes
- Could send individual messages
- Instead, use broadcast – more efficient, faster
- `int MPI_Bcast(void* buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm)`

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Gather

- All processes need to send same (similar) message to manager
- Could implement with each process calling `MPI_Send(…)` and manager looping through `MPI_Recv(…)`
- Instead, use gather operation – more efficient, faster
- Messages concatenated in rank order
- `int MPI_Gather(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`
- Note: `recvcount` = number of items received from each process, not total

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Gather

- Maybe some processes need to send longer messages than others
- Allow varying data count from each process with `MPI_Gatherv(…)`
- `int MPI_Gatherv(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int *recvcounts, int *displs, MPI_Datatype recvtype, int root, MPI_Comm comm)`
- `recvcounts` is array; entry `i` in `displs` array specifies displacement relative to `recvbuf[0]` at which to place data from corresponding process number

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Scatter

- Inverse of gather: split message into `NP` equal pieces, with `i`th segment sent to `i`th process in group
- `int MPI_Scatter(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`
- Send messages of varying sizes across processes in group: `MPI_Scatterv(…)`
- `int MPI_Scatterv(void* sendbuf, int *sendcounts, int *displs, MPI_datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, int root, MPI_Comm comm)`

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Reduce

- Perhaps we need to do sum of many subsums owned by all processors
- Perhaps we need to find maximum value of variable across all processors
- Perform global reduce operation across all group members
- `int MPI_Reduce(void* sendbuf, void* recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm)`

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Reduce: Predefined Operations

MPI_Op	Meaning	Allowed Types
MPI_MAX	Maximum	Integer, floating point
MPI_MIN	Minimum	Integer, floating point
MPI_SUM	Sum	Integer, floating point, complex
MPI_PROD	Product	Integer, floating point, complex
MPI_LAND	Logical and	Integer, logical
MPI_BAND	Bitwise and	Integer, logical
MPI_LOR	Logical or	Integer, logical
MPI_BOR	Bitwise or	Integer, logical
MPI_LXOR	Logical xor	Integer, logical
MPI_BXOR	Bitwise xor	Integer, logical
MPI_MAXLOC	Maximum value and location	*
MPI_MINLOC	Minimum value and location	*

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Reduce: Operations

- `MPI_MAXLOC` and `MPI_MINLOC`
  - Returns {max, min} and rank of first process with that value
  - Use with special MPI pair datatype arguments:
    - `MPI_FLOAT_INT` (`float` and `int`)
    - `MPI_DOUBLE_INT` (`double` and `int`)
    - `MPI_LONG_INT` (`long` and `int`)
    - `MPI_2INT` (pair of `int`)
  - See MPI standard for more details
- User-defined operations
  - Use `MPI_Op_create(…)` to create new operations
  - See MPI standard for more details

All- Operations

- Sometimes, may want to have result of gather, scatter, or reduce on all processes
- Gather operations
  - `int MPI_Allgather(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)`
  - `int MPI_Allgatherv(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int *recvcounts, int *displs, MPI_Datatype recvtype, MPI_Comm comm)`

All-to-All Scatter/Gather

- Extension of `Allgather` in which each process sends distinct data to each receiver
- Block `j` from process `i` is received by process `j` into `i`th block of `recvbuf`
- `int MPI_Alltoall(void* sendbuf, int sendcount, MPI_Datatype sendtype, void* recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)`
- Also corresponding `AlltoAllv` function available

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All-Reduce

- Same as MPI_Reduce except result appears on all processes
- `int MPI_Allreduce(void* sendbuf, void* recvbuf, int count, MPI_Datatype datatype, MPI_Op op, MPI_Comm comm)`

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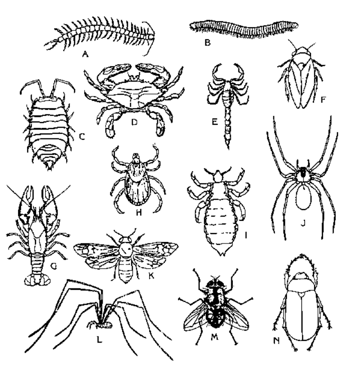
Barrier

- In algorithm, may need to synchronize processes
- Barrier blocks until all group members have called it
- `int MPI_Barrier(MPI_Comm comm)`



Source: http://www.uky.edu/Ag/Entomology/ythfacts/4h/unit1/i&tr.htm

V. DEBUGGING AND PERFORMANCE EVALUATION

V. Debugging and Performance Evaluation

- Common errors in parallel programs
- Debugging tools
- Overview of benchmarking and performance measurements

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Common Errors

- Program hangs
  - Send has no corresponding receive (or vice versa)
  - Send/receive pair do not match in source/recipient or tag
  - Condition you believe should occur does not occur
- Segmentation fault
  - Trying to access memory you are not allowed to access/ memory you should not have been allowed to access has been altered (e.g. array index out-of-bounds, uninitialized pointers, using non-pointer as pointer)
  - Trying to access a memory location in a way that is not allowed (e.g. overwrite a read-only location)

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Debugging Tools

- Debugging parallel codes is particularly difficult
- Problem: figuring out what happens on each node
- Solutions:
  - Print statements, I/O redirection into files belonging to each node
  - Debuggers compatible with MPI

Print Statement Debugging Method

- Each processor dumps print statements to `stdout` or into individual output files, e.g. `log.0001`, `log.0002`, etc.
- Advantage: easy to implement, independent of platform or available resources
- Disadvantage: time-consuming, extraneous information in log files

MPI-Compatible Debuggers

- TotalView
  - Commercial product, easy-to-use GUI
  - Installed on production systems such as Crays, probably not installed on local machines
- Free debuggers + `mpirun`
  - Use `mpirun` command and specify your favorite debugger, e.g. `mpirun -dbg=ddd -np 4 ./myprog`
  - This option available with MPICH and most other MPI implementations
  - Not as “pretty” as TotalView but it gets job done

Benchmarking and Performance

- Efficiency
- Scalability
- Performance modeling
- Example

Efficiency

- How well does parallel program perform compared to serial program (or parallel program on 1 processor)?

$$E_N = \frac{T_1}{N T_N}$$

- E = efficiency, N = # processors, T_p = time for p processors

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Efficiency

- Ideally, $E_N = 1$; realistically, $E_N < 1$.
- Factors influencing efficiency
  - Load balance (evenly distribute work for better efficiency)
  - Concurrency (minimize idle time on all processors)
  - Overhead (minimize work that serial computation would not do, e.g. communication)

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Scalability: Speedup

- How well does parallel program take advantage of additional processors?

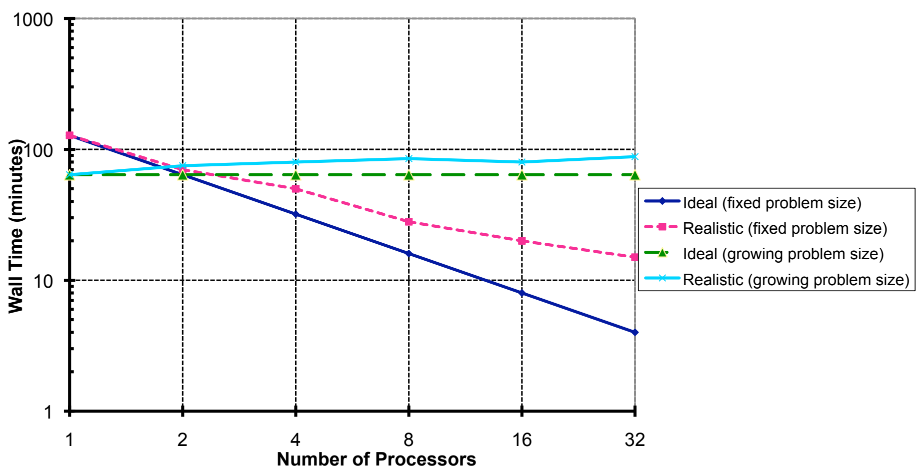
$$S_N = \frac{T_1}{T_N}$$

- S = speedup, N = # processors, T_p = time for p processors

Determining Scalability of Program

- How to measure scalability
  - Fixed problem size, measure T_N for different N's
  - Increase problem size proportional to N, compare T_N
- Repeat performance runs at least 3 times for each N (ideally >5 times)
- Plot on log-log graph; slope of line determines scalability

Scalability



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Performance Evaluation

- Create performance model

$$T_N = T_N^{\text{communication}} + T_N^{\text{computation}} + T_N^{\text{serial}}$$

- Examine parallel algorithm and figure out which parts fit in each category
- Perform least-squares fit with scalability data

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Benchmarking and Performance: Example

- Example of real program: three-tier parallel program from my dissertation
- The problem: Compute diffusion function
  - Compute *f* matrices, each matrix and each matrix entry independent of all others
  - Perform matrix-vector multiply for each matrix and take norm of result
  - Take weighted average of *f* results

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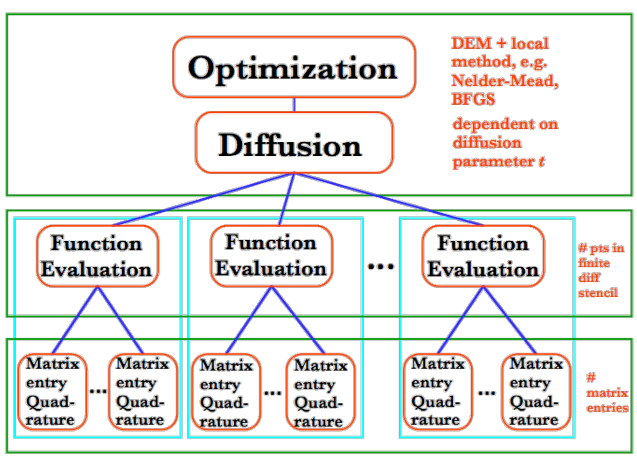
Example: Schematic Overview of Algorithm



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Example: Categorize Algorithm

Communication	Computation	Serial (Idle)
Manager: send information about computation to *All*		*Manager:* Initialize
	All: Compute matrix entries using quadrature	
Workers: Send matrix entries to *Drivers*		
	Drivers: Compute matrix/ vector multiply and norm	(*Worker* processes are idle)
Drivers: Send results to manager		
		Compute final function evaluation (*All* processes except *Manager* are idle)

Time →

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Example: Performance Evaluation

$$T_N = T_N^{\text{communication}} + T_N^{\text{computation}} + T_N^{\text{serial}}$$

For three-tier algorithm,

$$T_N = (3N + d - 1)t_s + P(N, f)t_{\text{quad}} + t_{\text{init}}$$

- N = # processors
- d = # drivers
- f = stencil size
- $P(N, f)$ = max # entries computed by 1 proc
- t_s = message startup time
- t_{quad} = avg time to compute one entry
- t_{init} = time spent by manager in serial

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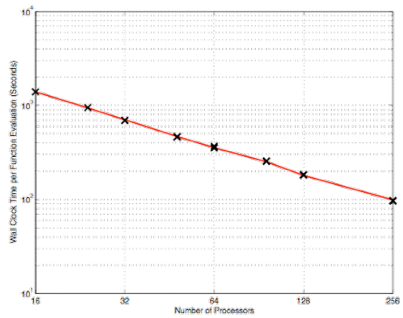
Example: Performance Evaluation

- Using least squares solve, we obtain

$$T_N = (3N + d - 1)\; 3.81077 \times 10^{-3} + P(N, f)\; 10.3311 + 3.91500 \quad \text{sec}$$



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  - MPI-2: http://www.mpi-forum.org/docs/mpi-20-html/mpi2-report.htm#Node0

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